



chain nodes :

19 21 22 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

6-19 8-19 16-19 21-22 24-25 24-26 26-28 26-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16  
16-17 17-18

exact/norm bonds :

13-14 13-18 14-15 15-16 16-17 17-18 21-22 24-25 24-26 26-28 26-27

exact bonds :

6-19 8-19 16-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 : 13 :

Connectivity :

27:1 E exact RC ring/chain 28:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 21:CLASS 22:CLASS  
23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 30:Atom